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Characteristics of Syngas Auto-ignition at High Pressure and Low Temperature Conditions with Thermal Inhomogeneities

Pinaki Pal[1,*], Andrew B. Mansfield[1], Margaret S. Wooldridge[1,2], Hong G. Im[3]

[1]*Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, United States*
[2]*Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI 48109, United States*
[3]*Clean Combustion Research Center, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia*

Abstract

Effects of thermal inhomogeneities on syngas auto-ignition at high-pressure low-temperature conditions, relevant to gas turbine operation, are investigated using detailed one-dimensional numerical simulations. Parametric tests are carried out for a range of thermodynamic conditions (T = 890-1100 K, P = 3-20 atm) and composition (Φ = 0.1, 0.5). Effects of global thermal gradients and localized thermal hot spots are studied. In the presence of a thermal gradient, the propagating reaction front transitions from spontaneous ignition to deflagration mode as the initial mean temperature decreases. The critical mean temperature separating the two distinct auto-ignition modes is computed using a predictive criterion and found to be consistent with front speed and Damkohler number analyses. The hot spot study reveals that compression heating of end-gas mixture by the propagating front is more pronounced at lower mean temperatures, significantly advancing the ignition delay. Moreover, the compression heating effect is dependent on the domain size.

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Keywords: Syngas, Auto-ignition, Deflagration, Spontaneous ignition, Strong and weak ignition

* Corresponding author. Tel.: +1 734 276 5896
E-mail address: pinaki@umich.edu

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1. Introduction

Syngas, primarily composed of hydrogen and carbon monoxide, provides an attractive choice as an alternative fuel for power generation applications, with a potential for near-zero pollutant emissions, including greenhouse gases such as carbon dioxide, when combined with carbon capture and sequestration methods. As such, there is growing interest in developing stationary power generation technology based on combustion of syngas derived from various conventional and alternative fuel sources. One of the critical challenges in this approach is that typical gas turbines in power plants are operated at high pressure (~ 20-30 bar) and intermediate/low temperature (< 1000 K) conditions, in which ignition and combustion characteristics of syngas are not well understood. A compilation of recent experimental and computational studies reported in Ref. [1] showed marked discrepancies between measurements and homogeneous chemical kinetic modeling predictions in the ignition delay, more pronounced as the initial temperature becomes lower. To reconcile the observed discrepancies, improved reaction mechanisms have been proposed [2], while some experimental studies suggested a possibility of alternative mechanisms attributed to different ignition behavior arising from the nonuniform temperature and mixture fields [3,4]. More recently, Mansfield and Wooldridge [5] experimentally investigated syngas auto-ignition regimes in a rapid compression machine, and found that the mixed ignition behavior at lower temperatures was strongly related to the increased sensitivity of ignition delay to thermal gradients. They proposed a criterion for the transition from strong to mixed ignition based on the computational study by Sankaran et al. [6]. While further experimental investigations are underway, additional systematic and detailed investigations are needed in order to provide general and comprehensive understanding of the effects of mixture inhomogeneities on ignition characteristics.

Therefore, the present study utilizes detailed numerical simulations to investigate the effects of the global and local temperature inhomogeneities on syngas auto-ignition behavior at temperature and pressure conditions relevant to practical applications. One-dimensional calculations are conducted for extensive parametric studies.

Model configuration and numerical setup

High fidelity numerical simulations are performed using S3D [7] as discussed in previous studies, incorporating detailed H_2/CO mechanism [8] with 12 species and 33 chemical reactions, and detailed thermodynamic and mixture-averaged transport properties. To allow extensive parametric studies, one-dimensional calculations are conducted with periodic boundary conditions to represent constant volume ignition process. A number of parametric conditions are considered at a mean temperature range of 890-1100 K, pressure range of 3-20 atm and fuel/air equivalence ratios of 0.1 and 0.5, with the H_2:CO molar ratio of 0.7:1. Sinusoidal temperature profiles with varying magnitudes of fluctuation and length scale are used to represent different bulk thermal gradients. Alternatively, to study the effect of localized hot spots, a gaussian temperature kernel with a size of 6 mm is imposed at the centre of the domain, with the surrounding mixture at a constant temperature. A grid resolution of 4.7 μm is used for all cases, allowing sufficient resolution for the thin propagating fronts. The initial flow conditions are quiescent.

2. Results and discussion

2.1. *Effects of bulk thermal gradient*

Figure 1(a) shows the temporal evolution of the front propagation speed (S_d) normalized by the laminar flame speed (S_L) based on the initial mean condition, for two initial mean temperatures at 1030 K and 910 K. The front speed curve is of typical ‘U-shape’ that represents a stabilized low speed front propagation

embedded in between the first ignition and final stage of fuel consumption, both exhibiting very high speeds due to nearly zero concentration gradients. For the high temperature case, the front speed is much greater than laminar flame speed due to the enhanced reactivity. Figure 1(b) shows the spatial profiles of the budget between the reaction and diffusion contributions to the net front propagation. For the initial temperature at 1030 K, the front propagation is dominated by reaction contribution, indicating that the front is in the spontaneous ignition regime. For the 910 K case, on the other hand, a much greater influence of diffusion is observed, suggesting that the front is in the deflagration regime.

Figure 2 shows the variation of the Damkohler number, *Da*, defined as the ratio of the positive peaks of reaction and diffusion of H_2 within the propagating reaction front, for different parametric conditions for the magnitude and length scale of the temperature fluctuation. With decreasing the mean temperature, *Da* approaches unity, indicating a shift from spontaneous ignition to deflagration. Following Ref. [6], the critical mean temperature separating homogeneous (chemistry-controlled) and inhomogeneous (reaction/transport balance) ignition phenomena is calculated for all the parametric sets using the following Sankaran number (Sa) criterion [6]:

$$\mathrm{Sa} = \beta \frac{S_L}{S_{sp}} = \beta S_L \left| \frac{d\tau_{\mathrm{ig}}}{dT} \frac{dT}{dx} \right| \leq 1 \tag{1}$$

which describes the effect of chemical kinetics, thermo-physical properties and system thermal characteristics on auto-ignition behavior. Strong ignition is encountered when the above inequality holds. At the strong ignition limit, the equality holds and a transition from strong to weak ignition occurs. A good correlation is found between this strong ignition limit and *Da* = 1.4.

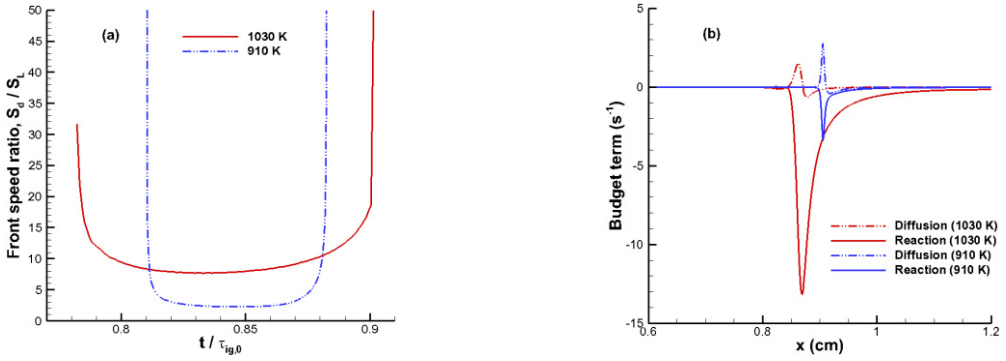

Figure 1: (a) Front speed versus time, and (b) spatial profiles of Y_{H2} budget terms in the front, for different initial mean temperatures, P_i = 20 atm, Φ = 0.5, T' = 10 K, L = 1.2 cm.

2.2. *Effects of thermal hot spots*

Figure 3 presents the evolution of temperature of the end gas mixture for two different initial mean temperatures in the presence of a thermal hot spot with a peak of 100 K above the mean. Evidently, at the lower mean temperature, the end gas auto-ignites significantly faster relative to the corresponding homogeneous condition. The front speed and *Da* analyses show that a deflagrative reaction front is formed for both cases. However, the front propagates farther towards the end of the domain for the lower temperature case (not shown here for brevity), resulting in enhanced compression heating of the end gas

(mixed ignition). This is due to the fact that the flame time scale, τ_f = L/ (2*S_d), L being the domain size, is much lower than the chemical time scale, τ_{chem} = end gas auto-ignition delay. On the other hand, for the higher mean temperature, $\tau_f > \tau_{chem}$, resulting in weaker compression heating effects (strong ignition).

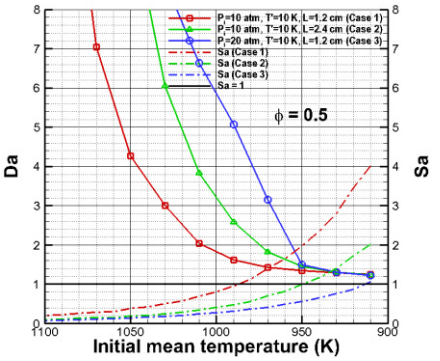

Figure 2: Front *Da* and *Sa* versus initial mean temperature (Φ = 0.5).

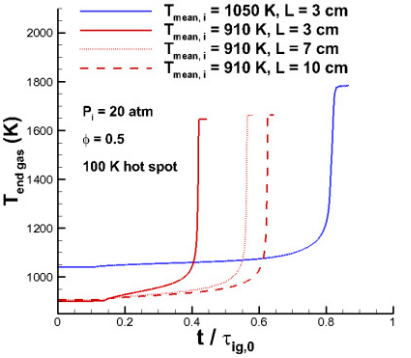

Figure 3: End gas temperature versus time for different initial mean temperatures and domain sizes.

In addition, a separate parametric study is carried out by keeping the initial mean temperature and hot spot strength constant and varying the domain size. It is observed that as the domain size is successively increased, compression heating by the propagating front becomes weaker due to an increase in τ_f and the final thermal runaway of the end gas gets retarded (as shown in Fig. 3).

3. Conclusions

The present numerical study shows that syngas auto-ignition is highly sensitive to thermal inhomogeneities at high pressure and low temperature conditions. Presence of thermal gradients and local hot spots can result in a variety of front propagation modes and ignition phenomena. A cut-off Damkohler number is proposed to distinguish between strong and mixed ignition. It is also shown that the compression heating of the end gas by front propagation is dependent on the size of the domain. Future work will aim to quantify the sensitivity of syngas auto-ignition to thermal non-uniformities in the T-P space considered here and extend the present study by incorporating the effects of turbulence, that can influence the development of thermal gradients, chemical kinetics and flame speeds significantly.

4. Acknowledgements

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